

10/ 070,804

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:sssptal202txn

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * Welcome to STN International * * * * *

NEWS 1 Web Page URLs for STN Seminar Schedule - N. America
NEWS 2 "Ask CAS" for self-help around the clock
NEWS 3 JAN 27 Source of Registration (SR) information in REGISTRY updated
and searchable
NEWS 4 JAN 27 A new search aid, the Company Name Thesaurus, available in
CA/CAPLUS
NEWS 5 FEB 05 German (DE) application and patent publication number format
changes
NEWS 6 MAR 03 MEDLINE and LMedline reloaded
NEWS 7 MAR 03 MEDLINE file segment of TOXCENTER reloaded
NEWS 8 MAR 03 FRANCEPAT now available on STN
NEWS 9 MAR 29 Pharmaceutical Substances (PS) now available on STN
NEWS 10 MAR 29 WPIFV now available on STN
NEWS 11 MAR 29 New monthly current-awareness alert (SDI) frequency in RAPRA
NEWS 12 APR 26 PROMT: New display field available
NEWS 13 APR 26 IFIPAT/IFIUDB/IFICDB: New super search and display field
available
NEWS 14 APR 26 LITAlert now available on STN
NEWS 15 APR 27 NLDB: New search and display fields available
NEWS 16 May 10 PROUSDDR now available on STN
NEWS 17 May 19 PROUSDDR: One FREE connect hour, per account, in both May
and June 2004
NEWS 18 May 12 EXTEND option available in structure searching
NEWS 19 May 12 Polymer links for the POLYLINK command completed in REGISTRY
NEWS 20 May 17 FRFULL now available on STN

NEWS EXPRESS MARCH 31 CURRENT WINDOWS VERSION IS V7.00A, CURRENT
MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
AND CURRENT DISCOVER FILE IS DATED 26 APRIL 2004
NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS INTER General Internet Information
NEWS LOGIN Welcome Banner and News Items
NEWS PHONE Direct Dial and Telecommunication Network Access to STN
NEWS WWW CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that
specific topic.

All use of STN is subject to the provisions of the STN Customer
agreement. Please note that this agreement limits use to scientific
research. Use for software development or design or implementation
of commercial gateways or other similar uses is prohibited and may
result in loss of user privileges and other penalties.

* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 16:32:28 ON 18 MAY 2004

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=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 16:32:33 ON 18 MAY 2004

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 17 MAY 2004 HIGHEST RN 682740-60-9

DICTIONARY FILE UPDATES: 17 MAY 2004 HIGHEST RN 682740-60-9

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

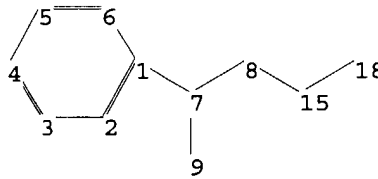
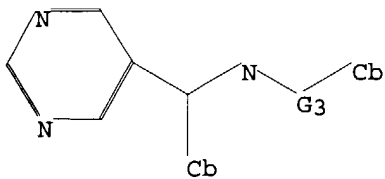
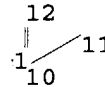
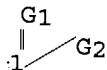
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:

<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

Uploading C:\STNEXP4\QUERIES\10070804.str



chain nodes :

7 8 9 10 11 12 15 18

ring nodes :

1 2 3 4 5 6

chain bonds :

1-7 7-8 7-9 8-15 10-11 10-12 15-18

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :

7-8 8-15 10-11 10-12 15-18

exact bonds :

1-7 7-9

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 :

G1:O,S

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G2:O,S,N

G3:SO2, [*1]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:Atom 10:CLASS
11:CLASS 12:CLASS 15:CLASS 18:Atom

Generic attributes :

9:

Saturation : Unsaturated

18:

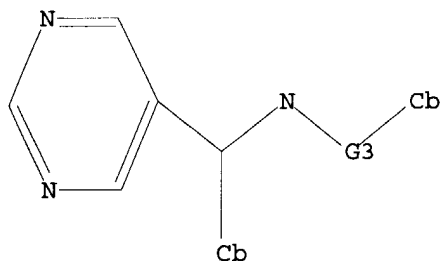
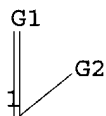
Saturation : Unsaturated

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



G1 O,S

G2 O,S,N

G3 SO2, [@1]

Structure attributes must be viewed using STN Express query preparation.

=> s l1 ful

FULL SEARCH INITIATED 16:33:04 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 25010 TO ITERATE

100.0% PROCESSED 25010 ITERATIONS

2 ANSWERS

SEARCH TIME: 00.00.01

L2 2 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE
ENTRY

TOTAL
SESSION

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FULL ESTIMATED COST

155.42

155.63

FILE 'CAPLUS' ENTERED AT 16:33:09 ON 18 MAY 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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FILE COVERS 1907 - 18 May 2004 VOL 140 ISS 21
FILE LAST UPDATED: 17 May 2004 (20040517/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 12

L3 1 L2

=> d 13 1- ibib abs hitstr

YOU HAVE REQUESTED DATA FROM 1 ANSWERS - CONTINUE? Y/(N):y

L3 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1999:765979 CAPLUS

DOCUMENT NUMBER: 132:46209

TITLE: A comparative molecular field analysis study of

obtusifoliol 14 α -methyl demethylase inhibitors

AUTHOR(S): Bargar, Tom M.; Secor, Jacob; Markley, Lowell D.;
Shaw, Brian A.; Erickson, Jon A.

CORPORATE SOURCE: Dow AgroSciences, Indianapolis, IN, 46268, USA

SOURCE: Pesticide Science (1999), 55(11), 1059-1069

CODEN: PSSCBG; ISSN: 0031-613X

PUBLISHER: John Wiley & Sons Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB This report describes the development of a Comparative Mol. Field Anal. (ComFA) model from a set of obtusifoliol 14 α -Me demethylase (DM) inhibitors to aid in the design of herbicides targeting sterol biosynthesis. ComFA is a three-dimensional (3-D) quant. structure-activity relationship (QSAR) method that is useful in the probing of receptor binding sites when exptl. structure data are unavailable. Conformational anal. and SAR of some rigid and active analogs were used to build the initial model using the active analog hypothesis. The model was subsequently used to design compds. that retain the active site shape requirements, but incorporate phys. properties that favor soil-applied herbicidal action. In addition, a second-generation ComFA model incorporating the newly designed inhibitors was developed and represents the current understanding of the DM binding site. This model was derived from a pharmacophore developed from two methods, the active analog approach as well as from the Catalyst program. The fact that two independent methods produced a similar pharmacophore strengthens the validity of the model.

IT 252895-58-2 252895-60-6

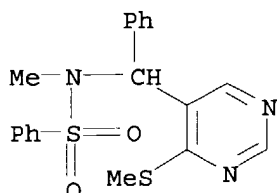
RL: AGR (Agricultural use); BAC (Biological activity or effector, except

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adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL
(Biological study); USES (Uses)
(herbicidal obtusifolios 14 α -Me demethylase inhibitor, used in
comparative mol. field anal. model)

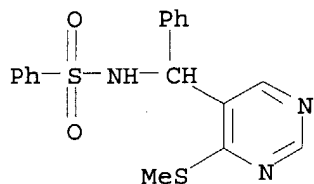
RN 252895-58-2 CAPLUS

CN Benzenesulfonamide, N-methyl-N-[[4-(methylthio)-5-
pyrimidinyl]phenylmethyl]- (9CI) (CA INDEX NAME)



RN 252895-60-6 CAPLUS

CN Benzenesulfonamide, N-[[4-(methylthio)-5-pyrimidinyl]phenylmethyl]- (9CI)
(CA INDEX NAME)



REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d his

(FILE 'HOME' ENTERED AT 16:32:28 ON 18 MAY 2004)

FILE 'REGISTRY' ENTERED AT 16:32:33 ON 18 MAY 2004

L1 STRUCTURE UPLOADED

L2 2 S L1 FUL

FILE 'CAPLUS' ENTERED AT 16:33:09 ON 18 MAY 2004

L3 1 S L2

=> log y

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
5.19	160.82

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
-0.69	-0.69

CA SUBSCRIBER PRICE

STN INTERNATIONAL LOGOFF AT 16:33:40 ON 18 MAY 2004